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Optimizing High-pressure Pair Distribution Function Measurements in Diamond Anvil Cells

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Pair distribution function (PDF) methods have great potential for the study of diverse high pressure phenomena. However, the measurement of high quality, high resolution x-ray PDF data (to $Q_{\max} > 20 \text{ \AA}^{-1}$) remains a technical challenge. Here we present an optimized approach to measuring high-pressure total scattering data for samples contained within a diamond anvil cell (DAC). This takes into account the coupled influences of instrument parameters (photon energy, detector type and positioning, beam size/shape, and focusing), pressure cell parameters (target pressure range, DAC type, diamonds, pressure transmitting media, backing plates, pressure calibration), and data reduction, on the resulting PDF. The efficacy of our approach is demonstrated by the high-quality, high-pressure PDFs obtained for representative materials spanning strongly and weakly scattering systems and crystalline and amorphous samples. These are the highest resolution high pressure PDFs reported to date, including for α -alumina (to $Q_{\max} = 20 \text{ \AA}^{-1}$), BaTiO_3 (to $Q_{\max} = 30 \text{ \AA}^{-1}$), and pressure amorphized zeolite (to $Q_{\max} = 20 \text{ \AA}^{-1}$).